

# GLOBAL DYNAMICS OF THE SMALLEST CHEMICAL REACTION SYSTEM WITH HOPF BIFURCATION

HAL L. SMITH\*

SCHOOL OF MATHEMATICAL AND STATISTICAL SCIENCES  
ARIZONA STATE UNIVERSITY  
TEMPE, AZ, USA 85287

**ABSTRACT.** The global behavior of solutions is described for the smallest chemical reaction system that exhibits a Hopf bifurcation, discovered in [7]. This three-dimensional system is a competitive system and a monotone cyclic feedback system. The Poincaré-Bendixson theory extends to such systems [6, 2, 3, 10] and a Bendixson criterion exists to rule out periodic orbits [4].

**Keywords:** competitive system, uniform persistence, monotone cyclic feedback system, compact attractor, periodic orbit, Bendixson criterion

## 1. INTRODUCTION AND MAIN RESULTS

In [7], Wilhelm and Heinrich discover the “smallest chemical reaction system” which may exhibit a Hopf bifurcation. Like the famous Lorenz system, it is a three dimensional system with only a single quadratic nonlinearity. In [8], they study the Hopf bifurcation in detail using center manifold and normal form techniques which establish the existence of a stable periodic orbit very near the bifurcation point. However, as they point out, their analysis does not preclude that chaotic behavior may not occur in this simple system. Sprott [12] has cataloged many other three dimensional systems with quadratic nonlinearities which can have chaotic dynamics. However, we will show that this particular chemical reaction system does not support chaos. We give a fairly complete analysis of the global dynamics of the system of ordinary differential equations studied in [8]. It is given by the following equations:

$$(1.1) \quad \begin{aligned} x' &= kx - k_2xy \\ y' &= k_5z - k_3y \\ z' &= k_4x - k_5z \end{aligned}$$

---

\*Supported by NSF Grant DMS-0918440.

where  $k_i > 0$ ,  $i = 2, 3, 4, 5$  and  $k = k_1A - k_4$  where  $A$  is the concentration of “the outer reactant of the autocatalytic reaction”. The  $k_i$  are rate constants and  $k$  need not be positive; see [7]. Variables  $x, y, z$  denote concentrations and therefore are nonnegative.

The scaling  $\bar{x} = x/a$ ,  $\bar{y} = y/b$ ,  $\bar{z} = z/c$  and the choice  $k_2b = 1$ ,  $k_5c = k_3b$ ,  $k_4a = k_5c$  leads to the system:

$$(1.2) \quad \begin{aligned} x' &= kx - xy \\ y' &= k_3(z - y) \\ z' &= k_5(x - z) \end{aligned}$$

where we have dropped the bar over variables for simplicity. Our focus is on the dynamics exhibited by (1.2) in the nonnegative octant  $\mathbb{R}_+^3$ .

System (1.2) is a competitive system because the signed incidence matrix of its Jacobian has a single loop with two positive feedbacks and one negative one:

$$x \xrightarrow{+} z \xrightarrow{+} y \xrightarrow{-} x$$

See [10, 3]; the change of variables  $z \rightarrow -z$  gives the system the canonical form with all off-diagonal entries of the Jacobian being non-positive. Since it is three dimensional, the celebrated Poincaré-Bendixon Theorem extends to its solutions by a result of M.W. Hirsch [2, 10, 3]: A compact omega or alpha limit set that contains no equilibrium is a periodic orbit. In fact, system (1.2) is also a monotone cyclic feedback system [6], for which the Poincaré-Bendixon Theorem also holds (regardless of the dimension of the system).

We note that 0 is the unique equilibrium of (1.2) if  $k \leq 0$ ; it is asymptotically stable if  $k \leq 0$  and unstable when  $k > 0$ . In the latter case, the stable manifold of 0 in  $\mathbb{R}_+^3$  is  $S = \{(x, y, x) \in \mathbb{R}_+^3 : x = 0\}$ . If  $k > 0$ , there is an additional equilibrium  $E = k(1, 1, 1)$  which is asymptotically stable if  $k < k_3 + k_5$  and unstable if  $k > k_3 + k_5$  with a pair of complex conjugate eigenvalues with positive real part and one negative eigenvalue.

Part (a) of the following result was proved in [8] using a linear Lyapunov function.

**Theorem 1.1.** *The following hold for (1.2):*

- (a) *If  $k \leq 0$ , every solution converges to 0.*
- (b) *If  $0 < k < k_3 + k_5$ , then every solution except those on  $S$  converge to  $E$ .*
- (c) *If  $k > k_3 + k_5$ , then every solution not starting on  $S$  or on the one-dimensional stable manifold of  $E$ , converges to a nontrivial*

*periodic orbit. At least one periodic orbit is orbitally asymptotically stable and the number of periodic orbits is finite.*

*Moreover, if  $k > 0$  then any solution not starting in  $S$  satisfies*

$$(1.3) \quad \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T u(s) ds = k, \quad u = x, y, z.$$

The main open problem concerning the dynamics of (1.2) is the number of periodic orbits in case (c). Numerical simulations suggest there is only one.

The geometry of the stable manifold of  $E$  is described in the following result. It is tangent at  $E$  to the eigenvector with sign pattern  $(+, +, -)$  and has certain monotonicity properties due to the monotonicity of the time-reversed system.

**Proposition 1.2.** *Let  $k > k_3 + k_5$ . Then the stable manifold of  $E$  in  $\mathbb{R}_+^3$  consists of  $E$  and two monotone solutions  $p_u(t) = (x_u(t), y_u(t), z_u(t))$ ,  $t \in [0, \infty)$  and  $p_l(t) = (x_l(t), y_l(t), z_l(t))$ ,  $t \in [0, \infty)$ .*

*$p_u$  satisfies  $p_u(0) = (x_u(0), 0, z_u(0))$  with  $0 < x_u(0) < k < z_u(0)$ ,  $p_u(\infty) = E$  and  $x_u, y_u$  are strictly increasing while  $z_u$  is strictly decreasing. Therefore, the graph of  $p_u$  belongs to  $[0, k] \times [0, k] \times [k, \infty)$ .*

*$p_l$  satisfies  $p_l(0) = (x_l(0), y_l(0), 0)$  with  $x_l(0), y_l(0) > k$ ,  $p_l(\infty) = E$  and  $x_l, y_l$  are strictly decreasing while  $z_l$  is strictly increasing. Therefore, the graph of  $p_l$  belongs to  $[k, \infty) \times [k, \infty) \times [0, k]$ .*

As a consequence of Proposition 1.2, the unstable manifold of 0 connects 0 to a nontrivial periodic solution in case (c) of Theorem 1.1; it cannot be a heteroclinic orbit connecting 0 to  $E$ .

**Theorem 1.3.** *System (1.2) has a non-empty compact invariant set  $A$  that attracts all bounded subsets of  $\mathbb{R}_+^3$ .*

*If  $k \leq 0$ , then  $A = \{0\}$ .*

*If  $k > 0$ . Then  $A \subset [0, M]^3$  where  $M = \frac{k(k+k_5)(k+k_3)}{k_3 k_5}$ .*

**Theorem 1.4.** *If  $k > 0$ , then (1.2) is uniformly persistent, i.e.,  $\exists \eta > 0$  such that:*

$$(1.4) \quad \min\{x(0), y(0), z(0)\} > 0 \Rightarrow \liminf_{t \rightarrow \infty} \min\{x(t), y(t), z(t)\} > \eta.$$

*The attractor  $A$  is the disjoint union  $A = \{0\} \cup C \cup A_1$  where:*

- (i)  $\{0\}$  attracts all bounded subsets of  $S$ .
- (ii)  $A_1$  is a compact invariant subset of the interior of  $\mathbb{R}_+^3$  that attracts all compact subsets of  $\mathbb{R}_+^3$  that do not intersect  $S$ .
- (iii)  $C$  is the one-dimensional unstable manifold of  $\{0\}$  which connects 0 to  $A_1$ .

## 2. PROOFS

*Proof.* Proof of Theorem 1.3. Let  $\phi(t, p)$  denote the solution of (1.2) which at  $t = 0$  is at  $p = (x(0), y(0), z(0))$ . If  $k \leq 0$ , then  $x' \leq 0$  and it is trivial to show that  $A = \{0\}$ .

Assume that  $k > 0$ . According to Theorem 2.33 in [11], we must show that (1.2) is point dissipative and for every bounded set  $B$  there exists  $t_r \geq 0$  such that  $\phi([t_r, \infty) \times B)$  is bounded.

We start by showing that it is point dissipative. If  $x(0) = 0$ , then  $x(t) = 0$  for all  $t$  and there exists  $\eta, \alpha > 0$  such that  $y(t) + z(t) \leq \eta(y(0) + z(0))e^{-\alpha t}$ . Assume that  $x(0) > 0$ . Then direct computation shows that

$$(2.1) \quad \begin{aligned} (y/x)' &\geq k_3(z/x) - (k + k_3)(y/x) \\ (z/x)' &\geq k_5 - (k + k_5)(z/x) \end{aligned}$$

It follows that  $(z/x)_\infty \geq \frac{k_5}{k+k_5}$  and  $(y/x)_\infty \geq \frac{k_3 k_5}{(k+k_3)(k+k_5)}$  where  $f_\infty = \liminf_{t \rightarrow \infty} f(t)$ . Consequently, for every  $\epsilon > 0$ , there exists  $t_0 > 0$  such that

$$x' = kx - x^2(y/x) \leq kx - m_\epsilon x^2, \quad t > t_0$$

where  $m_\epsilon = \frac{k_3 k_5}{(k+k_3)(k+k_5)} - \epsilon$ . Hence,  $x^\infty = \limsup_{t \rightarrow \infty} x(t) \leq k/m_\epsilon$  and, since  $\epsilon > 0$  is arbitrary,  $x^\infty \leq M$ . Using this estimate and the differential equation for  $z$  immediately yields  $z^\infty \leq M$ ; using this last estimate and the differential equation for  $y$  yields  $y^\infty \leq M$ . Thus, we have shown that all points are attracted to the bounded set  $[0, M]^3$  and (1.2) is point dissipative.

Now we identify a family of positively invariant bounded sets. Let  $0 < \sigma \leq \frac{k_5}{k+k_5}$ ,  $0 < \rho \leq \frac{k_3 \sigma}{k+k_3}$ , and  $K \geq k/\rho$ . Define

$$B_{(\sigma, \rho, K)} = \{(x, y, z) \in [0, K]^3 : x = 0 \text{ or } z/x \geq \sigma \text{ and } y/x \geq \rho\}$$

We claim that  $B_{(\sigma, \rho, K)}$  is positively invariant. Indeed, integrating the second inequality (2.1) leads to

$$(2.2) \quad (z/x)(t) \geq \frac{k_5}{k+k_5}(1 - e^{-(k+k_5)t}) + e^{-(k+k_5)t}(z/x)(0) \geq \sigma$$

for any solution starting in  $B_{(\sigma, \rho, K)}$  with  $x(0) \neq 0$ . Similarly, using that  $(z/x)(t) \geq \sigma$  in the first inequality (2.1) leads to

$$(y/x)(t) \geq \frac{k_3 \sigma}{k+k_3}(1 - e^{-(k+k_3)t}) + e^{-(k+k_3)t}(y/x)(0) \geq \rho.$$

As  $x' = kx - x^2(y/x) \leq x(k - \rho x) \leq 0$  when  $x = K$ ,  $z' = k_5(x - z) \leq 0$  when  $z = K$  and  $0 \leq x \leq K$ , and  $y' = k_3(z - y) \leq 0$  when  $y = K$  and  $0 \leq z \leq K$ , the positive invariance of  $B_{(\sigma, \rho, K)}$  follows.

Finally, we show that  $\forall L > 0$  there exists  $0 < \sigma < \frac{k_5}{k+k_5}$ ,  $0 < \rho < \frac{k_3\sigma}{k+k_3}$ , and  $K \geq k/\rho$  such that  $\phi(2, [0, L]^3) \subset B_{(\sigma, \rho, K)}$ . Since  $B_{(\sigma, \rho, K)}$  is bounded and positively invariant, this proves that  $\phi([2, \infty) \times [0, L]^3)$  is bounded. Hence, bounded sets have uniformly bounded orbits.

Let  $(x(0), y(0), z(0)) \in [0, L]^3$  and  $x(0) > 0$ . Integrating the second of (2.1) gives

$$\frac{z(t)}{x(t)} \geq \frac{k_5}{k+k_5}(1 - e^{-(k+k_5)t}), \quad t \geq 1.$$

Let  $\sigma$  be the right side of the above inequality and note that  $\sigma < \frac{k_5}{k+k_5}$ . Substituting this estimate into the first of (2.1) and integrating leads to

$$\frac{y(2)}{x(2)} \geq \frac{k_3\sigma}{k+k_3}(1 - e^{-(k+k_3)})$$

Let  $\rho$  be the right hand side of the above inequality and note that  $\rho < \frac{k_3\sigma}{k+k_3}$ . Now we can choose  $K > k/\rho$  so large that  $x(2), y(2), z(2) \leq K$  holds for every point  $(x(0), y(0), z(0)) \in [0, L]^3$ . It follows that for every point  $(x(0), y(0), z(0)) \in [0, L]^3$ , we have  $(x(2), y(2), z(2)) \in B_{(\sigma, \rho, K)}$ .  $\square$

*Proof.* Proof of Proposition 1.2. The time reversed system of (2.1) is a monotone dynamical system with respect to the partial order induced by the octant  $K = \{(x, y, z) : x, y \geq 0, z \leq 0\}$ . So we make use of Theorem 2.8 in [9]. By irreducibility of the Jacobian matrix at  $E$ , there is an eigenvector  $v \in K$  with nonzero components. Moreover, the unstable manifold of  $E$  for the time-reversed system consists of  $E$  and two strictly monotone trajectories  $P_u \in E - K$  and  $P_l \in E + K$  that are described in Theorem 2.8 in [9]. The monotone trajectory  $P_u$  must exit  $\mathbb{R}_+^3$  through the  $y = 0$  hyperplane because the derivative of  $y$  is negative and bounded away from zero.  $\square$

*Proof.* Proof of Theorem 1.4. We employ Theorem 8.17 in [11], using the notation developed there. Let  $p = (x, y, z) \in \mathbb{R}_+^3$  and  $\rho(p) = \min\{x, y, z\}$ .  $X_0 = \{p \in \mathbb{R}_+^3 : \rho(\phi(t, p)) = 0, t \geq 0\}$  consists of the stable manifold  $S$  of 0. The requisite compactness assumption (H) of Theorem 8.17 follows from Theorem 1.3.  $\Omega = \cup_{p \in X_0} \omega(p) = \{0\}$  where  $\omega(p)$  denotes the omega limit set of  $p$ .  $M \equiv \{0\}$  is obviously an acyclic covering of  $\Omega$  and it is an isolated invariant set in  $\mathbb{R}_+^3$  because 0 is a hyperbolic equilibrium (Hartman-Grobman Theorem). Finally,  $M$  is weakly  $\rho$ -repelling, meaning that there is no  $p \in \mathbb{R}_+^3$  such that  $\rho(p) > 0$  and  $\phi(t, p) \rightarrow M$  as  $t \rightarrow \infty$ . This follows because the stable manifold of 0 is exactly the  $x = 0$  facet  $S$  where  $\rho = 0$ . Consequently, we may

apply Theorem 8.17 in [11] to conclude that  $\phi$  is uniformly weakly  $\rho$ -persistent:  $\exists \eta > 0$  such that  $\rho(p) > 0 \Rightarrow \limsup_{t \rightarrow \infty} \rho(\phi(t, p)) > \eta$ . We conclude uniform strong persistence, i.e., replacing limsup by liminf in the above implication, by invoking Theorem 4.5 in [11].

The partition of the attractor  $A = \{0\} \cup C \cup A_1$  is a consequence of Theorem 5.7 in [11].  $\square$

*Proof.* Proof of Theorem 1.1. Part (a) was proved in [8]. Part (c) follows from Theorems 1.1 and 1.2 of [13] where we check that the determinant of the Jacobian at  $E$  is  $-kk_3k_5 < 0$ .

The final assertion uses the uniform persistence established in Theorem 1.4, which implies that the set  $D = [\eta, M]^3$  is an absorbing set for positive solutions of (1.2). Since  $\frac{1}{T} \int_0^T \frac{x'}{x} ds = \frac{1}{T} \ln(x(T)/x(0)) \rightarrow 0$  as  $T \rightarrow \infty$  because  $x$  is bounded and bounded away from zero, we see from the differential equation that  $\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T (k - y(s)) ds = 0$ . Indeed, this limit is uniform for all solutions starting in  $D$  because  $|\ln(x(T)/x(0))|$  is uniformly bounded on  $D$ . Thus,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T y(s) ds = k$$

uniformly for solutions in  $D$ . The other limits follow more easily and they too are uniform in  $D$ .

Part (b) is more technical. We use the geometric approach of ruling out periodic orbits developed in [4] which uses the second additive compound  $Df(p)^{[2]}$  of the Jacobian matrix  $Df(p)$ , where  $f(p)$  denotes the vector field (1.2):

$$Df(p)^{[2]} = \begin{pmatrix} k - y - k_3 & k_3 & 0 \\ 0 & k - y - k_5 & -x \\ -k_5 & 0 & -(k_3 + k_5) \end{pmatrix}$$

See, e.g., formula for  $Df(p)^{[2]}$  in appendix of [5]. As  $k < k_3 + k_5$ , we may find  $\epsilon \in (0, 1/2)$  such that  $k/(1 - 2\epsilon) < k_3 + k_5$ . Consider the  $3 \times 3$  matrix-valued function  $p \rightarrow A(p)$  where  $A(p)$  is a diagonal matrix with diagonal entries  $(1 - 2\epsilon)/x$ ,  $(1 - \epsilon)/x$ ,  $-1/k_5$ . Using the notation of [4], we compute the matrix function  $B(p) = A_f A^{-1} + A Df(p)^{[2]} A^{-1}$  where  $A_f$  is the directional derivative of  $A$  with respect to vector field  $f$ . We find that

$$(2.3) \quad B(p) = \begin{pmatrix} -k_3 & k_3 \frac{1-2\epsilon}{1-\epsilon} & 0 \\ 0 & -k_5 & k_5(1-\epsilon) \\ \frac{x}{1-2\epsilon} & 0 & -(k_3 + k_5) \end{pmatrix}$$

The Lozinskii measure  $\mu(B)$  relative to the norm  $|p| = \max\{|x|, |y|, |z|\}$  is (see pg 41 of [1]):

$$\mu(B) = \max\{-\epsilon k_3/(1 - \epsilon), -\epsilon k_5, \frac{x}{1 - 2\epsilon} - (k_3 + k_5)\}$$

Now we use that  $\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T x(s) ds = k$  is uniform for all orbits starting in the absorbing set  $B$  and that  $k/(1 - 2\epsilon) < k_3 + k_5$  to conclude that

$$\bar{q}_2 = \limsup_{t \rightarrow \infty} \sup_{p \in D} \frac{1}{T} \int_0^T \mu(B(\phi(s, p))) ds < 0.$$

Theorem 3.1 of [4] implies that there can be no nontrivial periodic orbit of (1.2). By the Poincaré-Bendixson Theorem for competitive three dimensional systems [2, 3, 10],  $E$  attracts all solutions not starting on  $S$ .  $\square$

## REFERENCES

- [1] W. Coppel, Stability and Asymptotic Behavior of Differential Equations, D.C. Heath, Boston, 1965.
- [2] M.W. Hirsch, Systems of Differential Equations that are Competitive or Cooperative. 1. limit sets., SIAM J. Math. Anal. 16 (1982), 167-179.
- [3] M. W. Hirsch and H. L. Smith, Monotone Dynamical Systems, in Handbook of Differential Equations, Ordinary Differential Equations (second volume), eds. A. Canada, P. Drabek, A. Fonda, Elsevier, 239-357, 2005.
- [4] M. Y. Li and J.S. Muldowney, A Geometric Approach to Global Stability Problems, SIAM J. Math. Anal. 27 (1996), 1070-1083.
- [5] M.Y. Li, H.L. Smith, and Liancheng Wang, Global Dynamics of an SEIR Epidemic Model with Vertical Transmission, SIAM J. Appl. Math. 62 (2001), 58-69.
- [6] J. Mallet-Paret and H. L. Smith, The Poincaré-Bendixson Theorem for monotone cyclic feedback systems, J. Dynamics & Diff. Eqns. 2, 1990, 367-421
- [7] T. Wilhelm and R. Heinrich, Smallest chemical reaction system with Hopf bifurcation, Journal of Mathematical Chemistry 17 (1995) 1-14
- [8] T. Wilhelm and R. Heinrich, Mathematical analysis of the smallest chemical reaction system with Hopf bifurcation, Journal of Mathematical Chemistry 19 (1996) 111 - 130
- [9] H. L. Smith, Systems of ordinary differential equations which generate an order preserving flow. a survey of results. SIAM Review 30 (1988) 87-113.
- [10] H. L. Smith, Monotone Dynamical Systems, AMS, Providence, 1995.
- [11] H.L. Smith and H.R. Thieme, Dynamical Systems and Population Persistence, Graduate Studies in Math. 118, Amer. Math. Soc. 2011.
- [12] J. Sprott, Some simple chaotic flows, Physical Review E 50 (1994), R647-R650.
- [13] H.-R. Zhu and H. L. Smith, Stable Periodic Orbits for a class of Three Dimensional Competitive Systems, J. of Diff. Eqns. 110 (1994) 143-156